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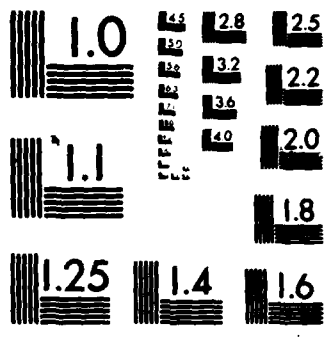JUN 82  G J IAFRATE

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## UTILIZATION OF QUANTUM DISTRIBUTION FUNCTIONS FOR ULTRA-SUBMICRON DEVICE TRANSPORT (U)

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### INTRODUCTION

As semiconductor technology continues to pursue the scaling-down of IC device dimensions into the submicron (less than ten thousand Angstroms) regime, many novel and interesting questions will emerge concerning the physics of charged particles in semiconductors. One of the more important topics to be considered is that of the appropriate transport (1) picture to be used for a given spatial and temporal regime. Moreover, from the point of view of device physics, it is most desirable to have a microscopic description of semiconductor transport which is computationally manageable or at least amenable to phenomenological treatment so that its properties can be meaningfully incorporated into device simulations. In this paper attention is focused on a useful transport methodology for the ultra-submicron regime. At present, military electronic devices with transit lengths in the ultra-submicron region are coming to fruition due to the advent of MBE (2) processing so that the need for an appropriate description of transport in this regime is indeed imperative.

Semiconductor transport in the ultra-submicron regime approaches the category of quantum transport. This is suggested by the fact that within the effective mass approximation the thermal deBroglie wavelength for electrons in semiconductors (see Fig. 1) is of the order of ultra-submicron dimensions. Whereas classical transport physics is based on the concept of a probability distribution function which is defined over the phase space of the system, in the quantum formulation of transport physics, the concept of a phase space distribution function is not possible inasmuch as the non-commutation of the position and momentum operators (the Heisenberg uncertainty principle) precludes the precise specification of a point in phase space. However, within the matrix formulation of quantum mechanics, it is possible to construct a "probability" density matrix which is often interpreted as the analog of the classical distribution function.
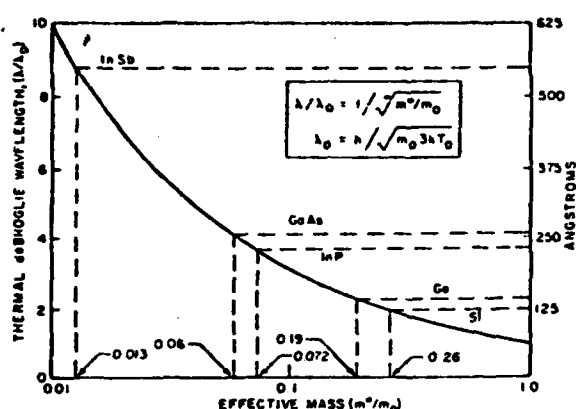
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Figure 1. Thermal deBroglie wavelength vs. effective mass

There is yet another approach to the formulation of quantum transport based on the concept of the Wigner distribution function (WDF) (3). This formalism is particularly attractive for use in ultra-submicron device transport in that it contains all of the quantum mechanical information about the state of the system yet has elements of the classical picture implicitly built in. Thus, the intent of this study is to explore the potential usefulness of the WDF as well as other possible quantum distribution functions for describing quantum (ultra-submicron) device transport in semiconductors. To this end we first review the salient features of the WDF and then discuss a new result, the derivation of the first three quantum moment equations using the WDF. It is shown that the moment equations contain quantum corrections to the classical moment equations; these quantum terms are non-negligible when the transit lengths are of the order of the carrier deBroglie wavelength.

## THE WIGNER DISTRIBUTION FUNCTION

The Wigner distribution function (3) is generally defined in terms of all the generalized coordinates and momenta of the system as

$$P_W(x_1 \ldots x_n, p_1 \ldots p_n) = \frac{1}{(2\pi\hbar)^n} \int_{-\infty}^{\infty} dy_1 \ldots dy_n \; \psi^*(x_1 + \frac{y_1}{2}, \ldots x_n$$

$$+ \frac{y_n}{2}) \; \psi (x_1 - \frac{y_1}{2}, \ldots x_n - \frac{y_2}{2}) \; e^{i(p_1 y_1 + \ldots + p_n y_n)/\hbar} .$$

(1)

However, for simplicity in this paper, we discuss the properties of a single coordinate and momentum WDF:

$$P_W(x,p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dy \, \Psi^*\left(x + \frac{y}{2}\right)\Psi\left(x - \frac{y}{2}\right) e^{ipy/\hbar} \qquad (2)$$

where $\Psi(x)$ represents the state of the system in the coordinate representation. Although we will be treating the WDF for the special case of pure states, the adaptation of this formalism to include mixed states is accomplished through the generalization

$$P_W(x,p) = \sum_n P_n \left[\frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dy \, \Psi_n^*\left(x + \frac{y}{2}\right)\Psi_n\left(x - \frac{y}{2}\right) e^{ipy/\hbar}\right]$$

where $P_n$ is the probability to be in state "n". (For example, for a system in contact with a heat bath at constant temperature, $P_n = e^{-E_n/kT}$.)

The distribution function of Eq. (2) has interesting properties in that the integration of this function over all momenta leads to the probability density in real space; conversely, the integration of this function over all coordinates leads to the probability density in momentum space. In mathematical terms,

$$\int_{-\infty}^{\infty} P_W(x,p) \, dp = \Psi^*(x)\Psi(x) \qquad (3a)$$

and

$$\int_{-\infty}^{\infty} P_W(x,p) \, dx = \phi^*(p)\phi(p), \qquad (3b)$$

where

$$\phi(p) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \Psi(x)dx.$$

It follows immediately from Eq. (3) that, for an observable $W(x,p)$ which is either a function of momentum operator alone or of position operator alone, or any additive combination therein, the expectation value of the observable is given by

$$\langle W \rangle = \iint W P_W(x,p) \, dx \, dp, \qquad (4)$$

which is analogous to the classical expression for the average value. Herein lies the interesting aspect of the Wigner distribution function; the

result of Eq. (4) suggests that it is possible to transfer many of the results of classical transport theory into quantum transport theory by simply replacing the classical distribution function by the Wigner distribution function. However, unlike the density matrix, the Wigner distribution function itself cannot be viewed as the quantum analog of the classical distribution function since it is generally not positive definite and non-unique [$P_W(x,p)$ of Eq. (2) is not the only bilinear expression (3-5) in $\Psi$ that satisfies Eq. (3)].

Further resemblance of the Wigner distribution function to the classical distribution function is apparent by examining the equation of time evolution for $P_W(x,p)$. Upon assuming that $\Psi(x)$ in Eq. (2) satisfies the Schrodinger equation for a system with hamiltonian $H = p^2/2m + V(x)$, it can be readily shown that $P_W(x,p)$ satisfies the equation

$$\partial P_W/\partial t + (p/m)\partial P_W/\partial x + \theta \cdot P_W = 0, \tag{5}$$

where

$$\theta \cdot P_W = -\frac{2}{\hbar} \sum_{n=0}^{\infty} (-1)^n \frac{(\hbar/2)^{2n+1}}{(2n+1)!} \frac{\partial^{2n+1} V(x)}{\partial x^{2n+1}} \frac{\partial^{2n+1} P_W(x,p)}{\partial p^{2n+1}} . \tag{6}$$

It is evident that in the limit $\hbar \to 0$, $\theta \cdot P_W$ in Eq. (6) becomes

$$\theta \cdot P_W = -(\partial V/\partial x)(\partial P_W/\partial p) \tag{7}$$

so that Eq. (5) reduces to the classical collisionless Boltzman equation.

The Wigner distribution function defined in Eq. (2) is derivable (8) from the Fourier inversion of the expectation value (with respect to state $\Psi(x)$) of the operator $e^{i(\tau\hat{p}+\theta\hat{x})}$ (here, $[\hat{x}$ and $\hat{p}]$ satisfy the commutation relation $[\hat{x},\hat{p}] = i\hbar$). As such,

$$P_W(x,p) = \frac{1}{4\pi^2} \iint C_W(\tau,\theta) e^{-i(\tau p+\theta x)} d\tau \, d\theta, \tag{8a}$$

where

$$C_W(\tau,\theta) = \int \Psi^*(x) e^{i(\tau\hat{p}+\theta\hat{x})} \Psi(x) \, dx, \tag{8b}$$

and the interval of integration is $(-\infty,\infty)$ unless otherwise specified. In order to show that the right-hand side of Eq. (8a) is indeed the Wigner distribution function as defined in Eq. (2), note, from the Baker-Hausdorff

theorem (9), that $e^{i(\tau\hat{p}+\theta\hat{x})}$ can be written

$$e^{i(\tau\hat{p}+\theta\hat{x})} = e^{i\tau\hat{p}/2}e^{i\theta\hat{x}}e^{i\tau\hat{p}/2} \,, \tag{9}$$

in which case $C_W(\tau,\theta)$ of Eq. (8b) becomes

$$C_W(\tau,\theta) = \int_{-\infty}^{\infty} [e^{-i\tau\hat{p}/2}\psi(x)]^* \; e^{i\theta\hat{x}} [e^{-i\tau\hat{p}/2}\psi(x)] \, dx \tag{10}$$

which further reduces to

$$C_W(\tau,\theta) = \int_{-\infty}^{\infty} \psi^*(x - \tfrac{1}{2}\tau h)e^{i\theta x}\psi(x + \tfrac{1}{2}\tau h) \, dx .. \tag{11}$$

Then, by inserting $C_W(\tau,\theta)$ of Eq. (11) into the right-hand side of Eq. (8a), integrating over the variable $\theta$ by using the relation

$$\int_{-\infty}^{\infty} e^{i\theta(x'-x'')} \, d\theta = 2\pi\delta(x'-x'') ,$$

and letting $\tau = y/h$, the desired result is obtained.

The method outlined above to arrive at the Wigner distribution function is based on the notion of a characteristic function. The characteristic function of an observable, A, with respect to state $|\psi\rangle$ (here, the Dirac notation is utilized for purposes of generality) is defined as

$$C_A(\xi) = \langle\psi|e^{i\xi\hat{A}}|\psi\rangle , \tag{12}$$

where $\xi$ is a real parameter. Assuming A to possess an eigenvalue spectrum given by $\hat{A}|A'\rangle = A'|A'\rangle$, $C_A(\xi)$ can be evaluated in the $A'$-representation as

$$C_A(\xi) = \int dA' \int dA'' \langle\psi|A'\rangle \langle A'|e^{i\xi A}|A''\rangle \langle A''|\psi\rangle . \tag{13}$$

Since $\langle A'|e^{i\xi\hat{A}}|A''\rangle = e^{i\xi A'}\delta(A' - A'')$ in the $A'$-representation, $C_A(\xi)$ in Eq. (13) reduces to

$$C_A(\xi) = \int dA'e^{i\xi A'}|\psi_{A'}|^2, \tag{14}$$

where $|\psi_{A'}|^2 = |\langle A'|\psi\rangle|^2 \equiv P(A')$, the probability distribution function for

measuring A' while in state $|\psi\rangle$. Hence, the characteristic function for $\hat{A}$ is the Fourier transform of the probability distribution function $P(A')$. Subsequent inversion of Eq. (14) above leads to

$$P(A') = \frac{1}{2\pi} \int C_A(\xi) e^{-i\xi A'} \, d\xi.. \tag{15}$$

The Wigner distribution function was derived by taking the Fourier transform of the characteristic function for $e^{i(\tau\hat{p}+\theta\hat{x})}$. In view of the connection between the probability distribution function and the characteristic function for a given observable, this approach seems to be a natural way of obtaining a distribution function for momentum and position. Unfortunately, the noncommutative nature of the two observables destroys the convenient probability interpretation of the characteristic function implicit in Eq. (15).

In order to demonstrate this point, assume the characteristic function for two noncommuting observables, $\hat{A}$ and $\hat{B}$, to be

$$C_{AB}(\xi_1\xi_2) = \langle \psi | e^{i(\xi_1\hat{A}+\xi_2\hat{B})} |\psi\rangle. \tag{16}$$

Observables $\hat{A}$ and $\hat{B}$ are assumed to have eigenvalue spectra

$$\hat{A}|A'\rangle = A'|A'\rangle, \quad \hat{B}|B'\rangle = B'|B'\rangle. \tag{17}$$

and are chosen so that $[\hat{A}, [\hat{A},\hat{B}]] = [\hat{B}, [\hat{A},\hat{B}]] = 0$.
This assumption is imposed so that the identity

$$e^{i(\xi_1\hat{A}+\xi_2\hat{B})} = e^{i\xi_1\hat{A}} e^{i\xi_2\hat{B}} e^{-\xi_1\xi_2[\hat{A},\hat{B}]/2} \tag{18}$$

may be used.

Inserting Eq. (18) into Eq. (16) while obtaining the matrix elements of $e^{i\xi_1 A}$ in the A-representation and $e^{i\xi_2 B}$ in the B-representation results in

$$C_{AB}(\xi_1\xi_2) = e^{-\xi_1\xi_2[\hat{A},\hat{B}]/2} \int dA' \int dB' \, e^{i(\xi_1 A'+\xi_2 B')} \langle\psi|A'\rangle\langle A'|B'\rangle\langle B'|\psi\rangle \tag{19}$$

In Eq. (19), it is assumed that $[A,B]$ is a c-number independent of the eigenvalues $A'$ and $B'$. We define $F(A',B')$, the generalized Wigner distribution function, to be

$$F(A',B') = \langle \Psi | A' \rangle \langle A' | B' \rangle \langle B' | \Psi \rangle, \tag{20}$$

so that

$$F(A',B') = \frac{1}{(2\pi)^2} \int d\xi_1 \int d\xi_2 \ e^{\xi_1 \xi_2 [\hat{A}, \hat{B}]/2} \ C_{AB}(\xi_1, \xi_2) e^{-i(\xi_1 A' + \xi_2 B')}. \tag{21}$$

It is evident from Eqs. (20,21) that

$$\int F(A',B') \ dA' \equiv |\langle B' | \Psi \rangle|^2 = \frac{1}{2\pi} \int d\xi_2 \ C_{AB}(0, \xi_2) e^{-i\xi_2 B'} \tag{22a}$$

and

$$\int F(A',B') \ dB' \equiv |\langle A' | \Psi \rangle|^2 = \frac{1}{2\pi} \int d\xi_1 \ C_{AB}(\xi_1, 0) e^{-i\xi_1 A'}. \tag{22b}$$

Thus, Eq. (21) establishes the relationship between the characteristic function for two arbitrary noncommuting observables and the generalized Wigner distribution function. The generalized distribution function has the essential properties of the conventional Wigner function in that an integration of the generalized function over the eigenvalue spectrum of one observable leads to the probability density in the canonically conjugate observable [Eq. (22)].

There is no simple probability interpretation of $F(A',B')$ in Eqs. (20, 21) because of the necessary overlap between the states of the noncommuting observables. However, if $\hat{A}$ and $\hat{B}$ are made to commute so that $|A'\rangle$ and $|B'\rangle$ are a common set of eigenvectors, then $F(A',B')$ reduces to the probability distribution function for $\hat{A}$ and $\hat{B}$.

Finally, it is noted that the conventional Wigner distribution function for observables $\hat{A}$ and $\hat{B}$ is obtained from

$$P_W(A',B') = \frac{1}{(2\pi)^2} \int d\xi_1 \int d\xi_2 \ C_{AB}(\xi_1, \xi_2) e^{-i(\xi_1 A' + \xi_2 B')}, \tag{23}$$

with $C_{AB}(\xi_1 \xi_2)$ defined in Eq. (16), whereas the alternative distribution function, $F(A',B')$, introduced in Eqs. (20,21) differs from the Wigner function due to the presence of the phase factor $e^{\xi_1 \xi_2 [\hat{A}, \hat{B}]/2}$ in the integrand of Eq. (21). For $\hat{A} = \hat{x}$ and $\hat{B} = \hat{p}$, $P_W(x,p)$ in Eq. (23) reduces to the Wigner function of Eq. (2), whereas $F(x,p)$ defined from Eq. (20) becomes

$$F(x,p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dy \ \Psi^*(x) \Psi(x - y) e^{ipy/\hbar} \equiv (2\pi\hbar)^{-1/2} \Psi^*(x) e^{ipx/\hbar} \phi(p), \tag{24}$$

where $\phi(p)$ is defined in Eq. (3b). It is evident that there is a family of functions which are bilinear in $\Psi$ yet satisfy the sum rules of Eqs. (3a,b).

There are some interesting questions to be resolved concerning the uniqueness and positive definiteness of Wigner-type quantum distribution functions. Nevertheless, these distribution functions serve a useful purpose for calculating quantum mechanical observables in transport (7) studies and numerous solid-state (10,11) problems.

## MOMENT EQUATIONS

In this section, we derive the first three moments of a "Wigner-Boltzmann"-like transport equation,

$$\frac{\partial P_w}{\partial t} + \frac{p}{m} \frac{\partial P_w}{\partial x} + \theta \cdot P_w = \left(\frac{\partial P_w}{\partial t}\right)_{coll.} \tag{25}$$

This equation was constructed to include an ad-hoc collision term which may not necessarily express the same phenomenology as that of the classical Boltzmann transport equation, since $P_w$ is not a true probability distribution function. These problems are conceptually reduced when dealing with moments in a relaxation approximation. The moment equations are obtained by multiplying Eq. (25) by an *appropriate* function of momentum, $\phi(p)$, and then integrating over all momenta to obtain:

$$\frac{\partial \langle \phi \rangle}{\partial t} + \frac{1}{m} \frac{\partial}{\partial x} \langle \phi p \rangle$$

$$- \sum_{n=0}^{\infty} \left(\frac{\hbar}{2i}\right) \frac{1}{(2n+1)!} \frac{\partial^{2n+1}}{\partial x^{2n+1}} V(x) \int \phi(p) \frac{\partial^{2n+1}}{\partial p^{2n+1}} P_w \, dp = \left\langle \phi \left(\frac{\partial P_w}{\partial t}\right)_{coll.} \right\rangle \tag{26}$$

where $\langle \ \rangle$ refers to an integration over momentum. In making the assumptions that $\phi(p)$ be an analytic function of momentum and that $P_w(x,p)$ vanish at the momentum limits, it follows that

$$\int \phi(p) \left(\frac{\partial^{2n+1}}{\partial p^{2n+1}} P_w\right) dp = (-1)^{2n+1} \int \left(\frac{\partial^{2n+1}}{\partial p^{2n+1}} \phi(p)\right) P_w \, dp \tag{27}$$

and that Eq. (26) becomes

$$\frac{\partial <\phi>}{\partial t} + \frac{1}{m} \frac{\partial}{\partial x} <\phi p>$$

$$+ \sum_{n=0}^{\infty} \left(\frac{\hbar}{2i}\right)^{2n} \frac{1}{(2n+1)!} \left(\frac{\partial^{2n+1}}{\partial x^{2n+1}} V(x)\right) < \frac{\partial^{2n+1}\phi}{\partial p^{2n+1}} > \; = \; < \phi \left(\frac{\partial P_w}{\partial t}\right)_{coll.} > . \qquad (28)$$

For specific values of $\phi(p) = p^0$, p, and $\frac{p^2}{2m}$, Eq. (28) becomes

$$\frac{\partial \rho}{\partial t} + \frac{1}{m} \frac{\partial}{\partial x} <p> = 0 , \qquad (29a)$$

$$\frac{\partial <p>}{\partial t} + \frac{1}{m} \frac{\partial}{\partial x} <p^2> + \rho \frac{\partial V}{\partial x} = <p \left(\frac{\partial P_w}{\partial t}\right)_{coll.} > , \qquad (29b)$$

$$\frac{1}{2m} \frac{\partial}{\partial t} <p^2> + \frac{1}{2m^2} \frac{\partial}{\partial x} <p^3> + \frac{<p>}{m} \frac{\partial V}{\partial x} = < \frac{p^2}{2m} \left(\frac{\partial P_w}{\partial t}\right)_{coll.} > \qquad (29c)$$

where upon reduction

$$<p^n> = \left(\frac{\hbar}{2i}\right)^n \sum_{j=0}^{n} (-1)^j \frac{n!}{(n-j)!j!} \frac{\partial^j \psi^*(x)}{\partial x^j} \frac{\partial^{n-j}\psi(x)}{\partial x^{n-j}} , \qquad (30)$$

thereby showing the dependence of $<p^n>$. For n = 0, 1, 2, 3 we show $<p^n>$ explicitly:

$$<p^0> = \psi^* \psi , \qquad <p^1> = \frac{\hbar}{2i} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right) , \qquad (31a)$$

$$<p^2> = \left(\frac{\hbar}{2i}\right)^2 \left(\psi^* \frac{\partial^2 \psi}{\partial x^2} - 2 \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} + \frac{\partial^2 \psi^*}{\partial x} \psi\right), \qquad (31b)$$

$$<p^3> = \left(\frac{\hbar}{2i}\right)^3 \left(\psi^* \frac{\partial^3 \psi}{\partial x^3} - 3 \frac{\partial \psi^*}{\partial x} \frac{\partial^2 \psi}{\partial x^2} + 3 \frac{\partial^2 \psi^*}{\partial x^2} \frac{\partial \psi}{\partial x} - \frac{\partial^3 \psi^*}{\partial x^3} \psi\right). \qquad (31c)$$

Note that use of Eqs. (31a) in Eq. (29a) results in the correct quantum mechanical continuity equation.

In order to see the transition between the quantum and classical regimes, we invoke a wavefunction of the form $\Psi(x,t) = A(x,t)e^{iS(x,t)/\hbar}$, and so

$$A^2(x,t) \equiv \Psi^*\Psi = \rho(x,t) \; , \quad \frac{1}{m} \frac{\partial S(x,t)}{\partial x} = v(x,t) \tag{32}$$

where $\rho(x,t)$ is the probability density and $v(x,t)$ is the ensemble velocity. Inserting the wavefunction of Eq. (32) into Eq. (31) results in

$$< p^0 > = \rho(x,t) \; , \quad < p^1 > = mv\rho \; , \tag{33a}$$

$$< p^2 > = (mv)^2 \rho - \frac{\hbar^2}{4m} \rho \frac{\partial^2}{\partial x^2} \ln\rho \; , \tag{33b}$$

$$< p^3 > = (mv)^3 \rho - \frac{\hbar}{4} \rho \left\{ 3mv \frac{\partial^2}{\partial x^2} \ln\rho + \frac{\partial^2}{\partial x^2} (mv) \right\} \; . \tag{33c}$$

It is evident from Eq. (33) that the terms possessing an explicit dependence on "$\hbar$" are the quantum corrections to the classical momentum-density moments. Furthermore, insertion of these momentum-moments into Eqs. (29) results in a set of moment equations which contain explicit quantum corrections as well. Of course, as $\hbar \to 0$, these moment equations reduce to the classical, zero temperature, moment equations.

The logarithmic derivative term appearing in Eqs. (33) is not uncommon; such a term appears in the real part of the Schrodinger equation when the wavefunction associated with Eq. (32) is used (9). In the limit where this term is negligible, the Schrodinger equation goes over to the Hamilton-Jacobi equation.

We have made order of magnitude estimates of the strengths of the quantum correction term appearing in Eq. (33). Using a Gaussian spatial variation for $\rho(x)$, and a thermal ensemble value for $mv^2$, typical of central valley GaAs electrons, we find that the quantum correction is substantial for distances of the order of $100°A$.

## SUMMARY

In this paper, we have puts forth a formalism for treating ultra-submicron device transport. The formalism results in a useful and attractive methodology for describing quantum device transport in that the theory is derived from a fully quantum mechanical representation, yet implicitly contains elements of the semiclassical semiconductor transport picture. The basic three semiconductor quantum transport equations were

*Will be expanded*

derived using the Wigner distribution function. These transport equations were shown to contain explicit quantum corrections; these quantum corrections are non-negligible when the transit lengths of the semiconductor device are of the order of the carrier deBroglie wavelength. Since the carrier deBroglie wavelength for carriers is of the order of hundreds of angstroms in III-V device materials of interest to the Army, the quantum description of transport as described here will play a vital role in predicting the electrical behavior of present and future generation ultra-submicron devices.

In future studies, we plan to expand our theoretical efforts to include device modeling of submicron and ultra-submicron semiconductor devices such as P-N junctions, planar doped barriers, and one- and two-dimensional superlattices; for these devices, it is clear that quantum transport will indeed be necessary to explain their semiconductor transport characteristics.

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